



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QT6  
Title : Crystal Structure Determination of a Blue Laccase from *Lentinus Tigrinus*  
Authors : Ferraroni, M.; Briganti, F.; Scozzafava, A.  
Deposited on : 2007-08-01  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

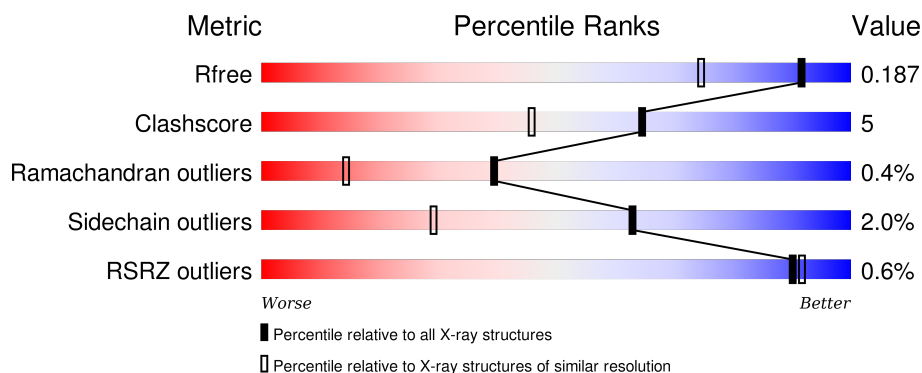
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	<div> <div></div> <div>91%</div> <div>8%</div> </div>
1	B	498	<div> <div></div> <div>92%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	TLA	A	3610	-	-	-	X
11	GOL	A	3611	-	-	-	X
2	BMA	B	709	-	-	-	X
4	NAG	A	605	-	-	-	X
5	MAN	A	3612	X	-	-	-
5	MAN	B	3711	X	-	-	-
7	CA	B	3712	-	-	-	X
9	PER	B	503	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10085 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

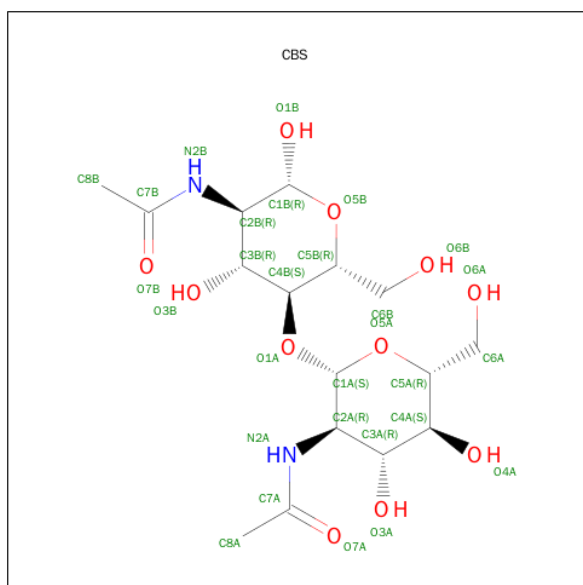
- Molecule 1 is a protein called Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	10	0
			3836	2430	641	750	15			
1	B	498	Total	C	N	O	S	0	8	0
			3828	2427	640	746	15			

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

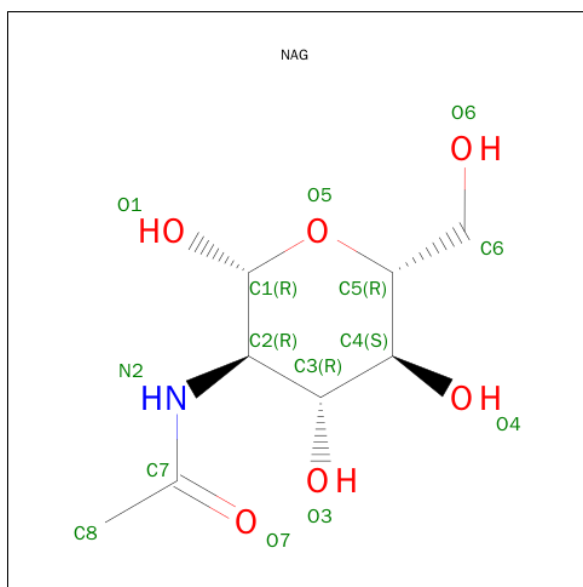
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			72	40	2	30		
2	B	5	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula:  $C_{16}H_{28}N_2O_{11}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	16	2	10		
3	B	1	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cu	0	0
			4	4		
6	A	4	Total	Cu	0	0
			4	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	5	Total	Ca	0	0
			5	5		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

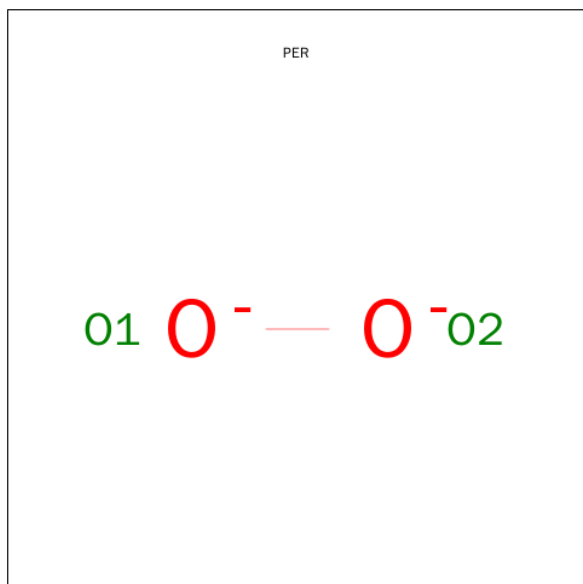
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		

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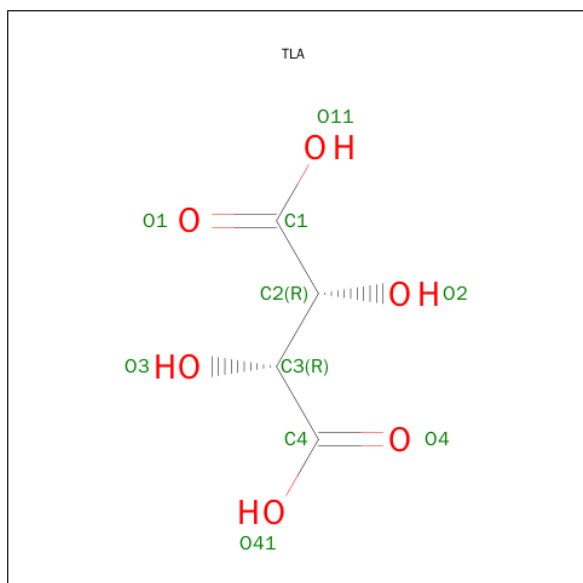
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Cl	0	0
			2	2		

- Molecule 9 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



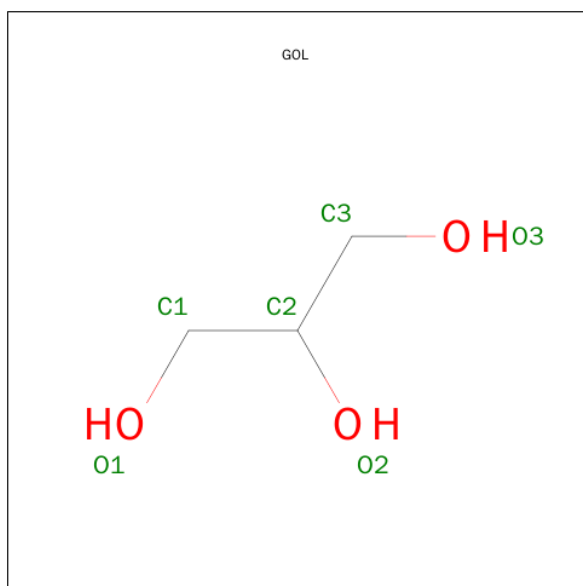
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O	0	0
			2	2		

- Molecule 10 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is water.

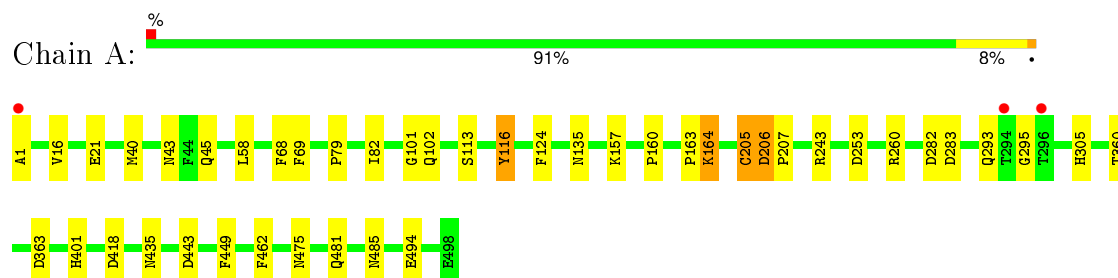
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1154	Total	O	0	6
			1160	1160		
12	B	980	Total	O	0	4
			984	984		



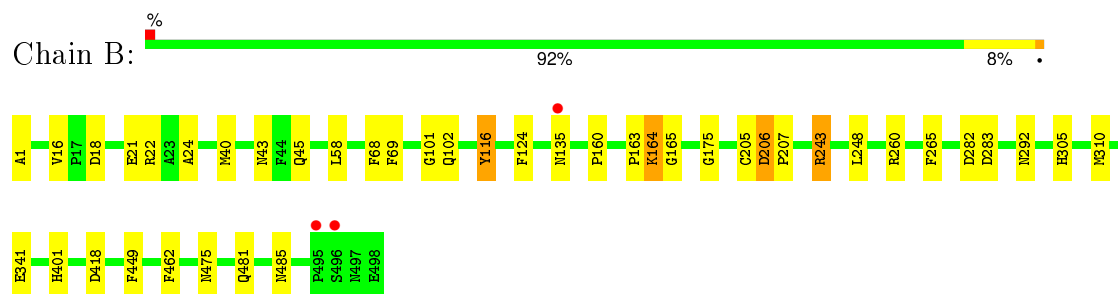
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Laccase



#### • Molecule 1: Laccase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.22Å 111.61Å 97.09Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 25.35 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.50) 98.0 (25.35-1.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.150 , 0.182 0.154 , 0.187	Depositor DCC
$R_{free}$ test set	922 reflections (0.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 210714 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CL, CA, PER, CBS, TLA, CU, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.71	0/4001	0.81	4/5497 (0.1%)
1	B	0.69	0/3983	0.76	2/5476 (0.0%)
All	All	0.70	0/7984	0.79	6/10973 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	A	253	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	205[A]	CYS	CA-CB-SG	-5.17	104.70	114.00
1	A	205[B]	CYS	CA-CB-SG	-5.17	104.70	114.00
1	B	260	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	243	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	HIS	Peptide
1	B	401	HIS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3836	0	3609	38	0
1	B	3828	0	3605	34	0
2	A	72	0	62	1	0
2	B	72	0	62	1	0
3	A	28	0	26	1	0
3	B	28	0	26	0	0
4	A	14	0	13	0	0
5	A	11	0	10	3	0
5	B	11	0	10	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	5	0	0	0	0
7	B	1	0	0	0	0
8	A	2	0	0	1	0
8	B	1	0	0	0	0
9	B	2	0	0	0	0
10	A	10	0	3	0	0
11	A	6	0	8	3	0
11	B	6	0	8	0	0
12	A	1160	0	0	15	2
12	B	984	0	0	12	3
All	All	10085	0	7442	78	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:H	1:A:164:LYS:HD3	1.18	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:HA	12:A:3936:HOH:O	1.58	1.03
1:A:157:LYS:HE2	12:A:3902:HOH:O	1.68	0.93
1:A:164:LYS:H	1:A:164:LYS:CD	1.81	0.89
1:B:164:LYS:H	1:B:164:LYS:CD	1.79	0.89
1:B:24:ALA:HA	12:B:3911:HOH:O	1.72	0.89
1:A:164:LYS:N	1:A:164:LYS:HD3	1.95	0.81
1:B:16:VAL:HG11	12:B:4412:HOH:O	1.82	0.80
1:B:164:LYS:H	1:B:164:LYS:HD2	1.47	0.80
1:B:22:ARG:NH2	12:B:3911:HOH:O	2.18	0.74
1:B:341:GLU:OE1	12:B:3883[A]:HOH:O	2.04	0.74
1:B:248:LEU:HG	12:B:3943:HOH:O	1.87	0.74
1:B:16:VAL:HG23	12:B:4154:HOH:O	1.89	0.73
1:A:16:VAL:HG12	1:A:21:GLU:HA	1.70	0.72
11:A:3611:GOL:H31	12:A:4383:HOH:O	1.91	0.71
1:A:260:ARG:NE	1:A:293[A]:GLN:HG2	2.05	0.71
1:B:40[B]:MET:HE2	1:B:101:GLY:HA2	1.73	0.70
1:B:43:ASN:ND2	1:B:45:GLN:HE21	1.90	0.68
1:B:164:LYS:HD2	1:B:164:LYS:N	2.04	0.68
1:B:16:VAL:HG12	1:B:21:GLU:HA	1.74	0.68
5:A:3612:MAN:C1	12:A:4863:HOH:O	2.43	0.66
1:A:16:VAL:HG12	1:A:21:GLU:CA	2.25	0.65
1:A:16:VAL:HG23	12:A:4328:HOH:O	1.96	0.65
1:A:157:LYS:CE	12:A:3902:HOH:O	2.36	0.65
1:A:16:VAL:HG11	12:A:4719:HOH:O	1.97	0.65
1:B:1:ALA:HA	12:B:3722:HOH:O	1.98	0.62
1:B:305:HIS:HE1	12:B:4045:HOH:O	1.82	0.62
1:A:164:LYS:N	1:A:164:LYS:CD	2.60	0.61
3:A:604:CBS:H61A	12:A:4332:HOH:O	2.01	0.61
1:B:164:LYS:NZ	12:B:3884:HOH:O	2.29	0.60
1:A:305:HIS:HE1	12:A:4177:HOH:O	1.84	0.60
1:A:43:ASN:HD21	1:A:45:GLN:HE21	1.48	0.59
1:B:305:HIS:HD2	1:B:418:ASP:O	1.86	0.59
1:A:305:HIS:HD2	1:A:418:ASP:O	1.85	0.59
1:B:16:VAL:HG12	1:B:21:GLU:CA	2.32	0.58
1:A:40[B]:MET:HE2	1:A:101:GLY:HA2	1.86	0.58
1:A:69:PHE:H	1:A:102:GLN:HE22	1.50	0.58
1:A:293[A]:GLN:HG3	12:A:4206:HOH:O	2.03	0.57
1:B:164:LYS:H	1:B:164:LYS:CE	2.17	0.57
1:B:116:TYR:CE1	1:B:205[A]:CYS:SG	2.98	0.57
1:A:113:SER:H	11:A:3611:GOL:C3	2.18	0.56
1:B:69:PHE:H	1:B:102:GLN:HE22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:HB2	8:A:3720:CL:CL	2.43	0.55
1:A:113:SER:H	11:A:3611:GOL:H32	1.72	0.55
2:B:707:BMA:H62	12:B:4698:HOH:O	2.07	0.54
1:A:282:ASP:O	1:A:283:ASP:HB2	2.09	0.53
1:A:160:PRO:HG2	1:A:164:LYS:HD2	1.91	0.51
1:B:160:PRO:HG2	1:B:164:LYS:CE	2.40	0.51
1:A:163:PRO:HA	1:A:164:LYS:HD3	1.93	0.51
1:B:163:PRO:HA	1:B:164:LYS:HE3	1.94	0.50
1:A:481:GLN:HE21	1:A:485:ASN:HD21	1.60	0.49
1:B:43:ASN:HD21	1:B:45:GLN:HE21	1.61	0.49
1:B:310[A]:MET:HE2	12:B:4483:HOH:O	2.12	0.49
5:A:3612:MAN:O6	12:A:4858[A]:HOH:O	2.20	0.48
1:B:16:VAL:HG23	1:B:16:VAL:O	2.14	0.48
1:B:160:PRO:HG2	1:B:164:LYS:HE3	1.96	0.47
1:A:116:TYR:CE1	1:A:205[A]:CYS:SG	3.07	0.47
1:A:481:GLN:HE21	1:A:485:ASN:ND2	2.14	0.46
1:A:360[B]:THR:HG23	1:A:363:ASP:H	1.81	0.45
1:A:135:ASN:ND2	12:A:3930:HOH:O	2.31	0.44
1:B:68:PHE:HA	1:B:102:GLN:HE22	1.84	0.43
1:B:165:GLY:HA2	1:B:265:PHE:CE2	2.55	0.42
1:A:295:GLY:HA3	12:A:4366:HOH:O	2.18	0.42
1:A:79:PRO:HB2	1:A:82:ILE:HB	2.02	0.42
1:B:475:ASN:ND2	12:B:4462:HOH:O	2.52	0.42
2:A:607:BMA:O3	5:A:3612:MAN:C1	2.68	0.42
1:A:16:VAL:HG13	12:A:4408:HOH:O	2.19	0.42
1:A:43:ASN:ND2	1:A:45:GLN:HE21	2.15	0.42
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.50	0.42
1:B:164:LYS:H	1:B:164:LYS:HE3	1.83	0.41
1:A:260:ARG:CD	1:A:293[A]:GLN:HG2	2.50	0.41
1:A:40[B]:MET:CE	12:A:4679:HOH:O	2.68	0.41
1:B:206:ASP:HB3	1:B:207:PRO:CD	2.50	0.41
1:A:68:PHE:HA	1:A:102:GLN:HE22	1.86	0.41
1:B:18:ASP:HA	1:B:175:GLY:O	2.21	0.40
1:B:282:ASP:O	1:B:283:ASP:HB2	2.22	0.40
1:B:481:GLN:HE21	1:B:485:ASN:HD21	1.69	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:3887:HOH:O	12:B:4541:HOH:O[2_745]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:4834:HOH:O	12:B:4203:HOH:O[2_645]	2.05	0.15
12:A:3937:HOH:O	12:B:4054:HOH:O[2_645]	2.07	0.13

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	505/498 (101%)	492 (97%)	11 (2%)	2 (0%)	39	14
1	B	504/498 (101%)	489 (97%)	13 (3%)	2 (0%)	39	14
All	All	1009/996 (101%)	981 (97%)	24 (2%)	4 (0%)	39	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	B	206	ASP
1	B	58	LEU
1	A	58	LEU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/420 (102%)	419 (98%)	10 (2%)	58	24
1	B	427/420 (102%)	419 (98%)	8 (2%)	65	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	856/840 (102%)	838 (98%)	18 (2%)	63	27

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	TYR
1	A	124	PHE
1	A	164	LYS
1	A	243	ARG
1	A	435	ASN
1	A	449	PHE
1	A	462	PHE
1	A	475	ASN
1	A	494[A]	GLU
1	A	494[B]	GLU
1	B	116	TYR
1	B	124	PHE
1	B	135	ASN
1	B	164	LYS
1	B	243	ARG
1	B	292	ASN
1	B	449	PHE
1	B	462	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	43	ASN
1	A	70	GLN
1	A	91	ASN
1	A	102	GLN
1	A	305	HIS
1	A	315	ASN
1	A	485	ASN
1	B	39	ASN
1	B	43	ASN
1	B	70	GLN
1	B	91	ASN
1	B	102	GLN
1	B	135	ASN

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Mol	Chain	Res	Type
1	B	292	ASN
1	B	305	HIS
1	B	315	ASN
1	B	485	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CBS	A	603	1,2	29,29,30	0.75	0	36,41,43	1.46	6 (16%)
2	BMA	A	606	2	11,11,12	0.39	0	14,15,17	1.58	1 (7%)
2	BMA	A	607	2	11,11,12	0.74	0	14,15,17	4.69	4 (28%)
2	BMA	A	608	2	11,11,12	0.64	0	14,15,17	2.46	3 (21%)
2	BMA	A	609	2	11,11,12	0.75	0	14,15,17	3.88	3 (21%)
2	CBS	B	704	1,2	29,29,30	0.68	0	36,41,43	1.54	9 (25%)
2	BMA	B	706	2	11,11,12	0.46	0	14,15,17	1.39	2 (14%)
2	BMA	B	707	2	11,11,12	0.54	0	14,15,17	2.21	3 (21%)
2	BMA	B	708	2	11,11,12	0.60	0	14,15,17	3.97	5 (35%)
2	BMA	B	709	2	11,11,12	0.57	0	14,15,17	2.87	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBS	A	603	1,2	-	0/16/53/56	0/2/2/2
2	BMA	A	606	2	-	0/2/19/22	0/1/1/1
2	BMA	A	607	2	-	0/2/19/22	0/1/1/1
2	BMA	A	608	2	-	0/2/19/22	0/1/1/1
2	BMA	A	609	2	-	0/2/19/22	0/1/1/1
2	CBS	B	704	1,2	-	0/16/53/56	0/2/2/2
2	BMA	B	706	2	-	0/2/19/22	0/1/1/1
2	BMA	B	707	2	-	0/2/19/22	0/1/1/1
2	BMA	B	708	2	-	0/2/19/22	0/1/1/1
2	BMA	B	709	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	BMA	C1-C2-C3	-12.00	95.35	109.54
2	A	607	BMA	C1-O5-C5	-11.55	97.59	112.25
2	A	609	BMA	C1-C2-C3	-10.39	97.24	109.54
2	B	708	BMA	C1-O5-C5	-9.52	100.17	112.25
2	B	708	BMA	C1-C2-C3	-9.05	98.83	109.54
2	A	609	BMA	C1-O5-C5	-8.96	100.88	112.25
2	B	709	BMA	C1-O5-C5	-7.43	102.81	112.25
2	B	709	BMA	C1-C2-C3	-6.96	101.31	109.54
2	A	608	BMA	C1-O5-C5	-6.52	103.97	112.25
2	A	606	BMA	O3-C3-C4	-4.97	99.14	110.34
2	B	707	BMA	C1-O5-C5	-4.74	106.23	112.25
2	A	608	BMA	C1-C2-C3	-4.70	103.98	109.54
2	B	707	BMA	C1-C2-C3	-4.52	104.20	109.54
2	B	704	CBS	O1A-C1A-O5A	-3.56	101.67	110.68
2	A	603	CBS	O1A-C1A-O5A	-3.23	102.51	110.68
2	B	706	BMA	O3-C3-C4	-2.68	104.31	110.34
2	B	704	CBS	O1A-C4B-C5B	-2.61	102.46	109.32
2	B	704	CBS	O7B-C7B-C8B	-2.39	117.68	122.06
2	A	603	CBS	C1A-C2A-N2A	-2.33	106.62	111.01
2	B	704	CBS	C8A-C7A-N2A	-2.30	111.71	116.11
2	B	704	CBS	C1A-C2A-N2A	-2.19	106.89	111.01
2	B	704	CBS	C1A-O1A-C4B	-2.05	112.65	118.01
2	A	603	CBS	C3B-C4B-C5B	-2.02	106.26	110.84
2	B	708	BMA	O6-C6-C5	-2.00	104.72	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	CBS	O1A-C4B-C3B	2.02	112.38	107.17
2	A	603	CBS	O5B-C5B-C6B	2.03	111.75	107.35
2	A	608	BMA	C3-C4-C5	2.21	114.04	110.20
2	A	603	CBS	O1A-C4B-C3B	2.40	113.37	107.17
2	B	708	BMA	O5-C5-C6	2.43	112.61	107.35
2	A	607	BMA	O5-C5-C6	2.51	112.79	107.35
2	A	609	BMA	C3-C4-C5	2.75	115.00	110.20
2	A	607	BMA	O2-C2-C1	2.82	114.87	109.21
2	B	704	CBS	O7B-C7B-N2B	3.07	128.12	121.86
2	B	707	BMA	C3-C4-C5	3.41	116.15	110.20
2	B	706	BMA	O3-C3-C2	3.42	116.19	110.00
2	B	704	CBS	C1B-O5B-C5B	3.69	116.93	112.25
2	A	603	CBS	C1B-O5B-C5B	4.58	118.06	112.25
2	B	708	BMA	O3-C3-C2	5.57	120.06	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	607	BMA	1	0
2	B	707	BMA	1	0

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 17 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	TLA	A	3610	7	3,9,9	0.49	0	6,12,12	1.15	1 (16%)
11	GOL	A	3611	-	5,5,5	0.44	0	5,5,5	0.64	0
5	MAN	A	3612	-	11,11,12	0.73	0	14,15,17	1.46	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CBS	A	604	1	29,29,30	0.59	0	36,41,43	1.18	4 (11%)
4	NAG	A	605	1,7	14,14,15	0.81	0	15,19,21	1.47	4 (26%)
11	GOL	B	3710	-	5,5,5	0.41	0	5,5,5	0.70	0
5	MAN	B	3711	-	11,11,12	0.60	0	14,15,17	0.84	0
9	PER	B	503	6	0,1,1	0.00	-	0,0,0	0.00	-
3	CBS	B	705	1	29,29,30	0.41	0	36,41,43	0.88	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	TLA	A	3610	7	-	0/4/12/12	0/0/0/0
11	GOL	A	3611	-	-	0/4/4/4	0/0/0/0
5	MAN	A	3612	-	1/1/4/5	0/2/19/22	0/1/1/1
3	CBS	A	604	1	-	0/16/53/56	0/2/2/2
4	NAG	A	605	1,7	-	0/6/23/26	0/1/1/1
11	GOL	B	3710	-	-	0/4/4/4	0/0/0/0
5	MAN	B	3711	-	1/1/4/5	0/2/19/22	0/1/1/1
9	PER	B	503	6	-	0/0/0/0	0/0/0/0
3	CBS	B	705	1	-	0/16/53/56	0/2/2/2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	NAG	C8-C7-N2	-2.47	111.38	116.11
4	A	605	NAG	C2-N2-C7	-2.32	120.06	123.04
3	B	705	CBS	C1A-O1A-C4B	-2.29	112.02	118.01
4	A	605	NAG	O4-C4-C3	-2.19	105.41	110.34
3	A	604	CBS	O3A-C3A-C2A	-2.18	105.21	109.66
3	A	604	CBS	C3A-C2A-N2A	-2.08	106.37	110.66
10	A	3610	TLA	C1-C2-C3	-2.02	109.21	113.35
5	A	3612	MAN	C3-C4-C5	2.25	114.12	110.20
3	A	604	CBS	C3A-C4A-C5A	2.63	114.79	110.20
4	A	605	NAG	O3-C3-C2	2.97	115.00	109.11
5	A	3612	MAN	C1-C2-C3	3.44	113.61	109.54
3	A	604	CBS	C4A-C3A-C2A	3.48	115.26	110.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	3711	MAN	C5
5	A	3612	MAN	C5

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	3611	GOL	3	0
5	A	3612	MAN	3	0
3	A	604	CBS	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	498/498 (100%)	-0.35	3 (0%) 90 92	15, 19, 27, 35	0
1	B	498/498 (100%)	-0.10	3 (0%) 90 92	16, 23, 33, 40	0
All	All	996/996 (100%)	-0.23	6 (0%) 90 92	15, 20, 30, 40	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	THR	4.7
1	B	495	PRO	3.6
1	B	135	ASN	3.0
1	A	1	ALA	2.8
1	B	496	SER	2.5
1	A	294	THR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	B	709	11/12	0.73	0.20	5.27	43,46,48,48	0
2	CBS	B	704	28/29	0.91	0.09	0.26	19,22,26,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CBS	A	603	28/29	0.96	0.06	-0.42	16,18,20,21	0
2	BMA	A	607	11/12	0.79	0.22	-	35,37,43,49	0
2	BMA	A	606	11/12	0.89	0.13	-	24,28,33,34	0
2	BMA	B	707	11/12	0.69	0.28	-	48,51,54,57	0
2	BMA	B	708	11/12	0.69	0.25	-	45,48,49,51	0
2	BMA	A	609	11/12	0.76	0.20	-	40,42,47,49	0
2	BMA	B	706	11/12	0.88	0.18	-	31,37,40,46	0
2	BMA	A	608	11/12	0.67	0.28	-	51,53,55,56	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PER	B	503	2/2	0.93	0.12	9.47	23,23,23,33	2
11	GOL	A	3611	6/6	0.84	0.14	5.88	25,32,34,36	0
4	NAG	A	605	14/15	0.83	0.21	4.22	21,30,36,41	0
7	CA	B	3712	1/1	0.99	0.11	2.32	19,19,19,19	1
10	TLA	A	3610	10/10	0.96	0.10	2.19	21,23,25,29	0
3	CBS	B	705	28/29	0.73	0.17	1.87	31,38,47,49	0
3	CBS	A	604	28/29	0.92	0.10	1.58	18,24,34,39	0
8	CL	A	3720	1/1	1.00	0.09	0.56	37,37,37,37	0
7	CA	A	3716	1/1	1.00	0.04	-1.31	18,18,18,18	0
6	CU	A	502	1/1	1.00	0.03	-4.18	21,21,21,21	1
6	CU	A	501	1/1	1.00	0.03	-4.77	22,22,22,22	1
6	CU	A	499	1/1	1.00	0.03	-4.84	19,19,19,19	1
6	CU	B	502	1/1	1.00	0.02	-5.52	24,24,24,24	1
6	CU	B	499	1/1	1.00	0.02	-6.25	24,24,24,24	1
8	CL	A	3719	1/1	1.00	0.05	-6.48	29,29,29,29	0
8	CL	B	3718	1/1	1.00	0.05	-6.98	32,32,32,32	0
6	CU	B	501	1/1	0.99	0.03	-7.46	26,26,26,26	1
7	CA	A	3715	1/1	1.00	0.03	-	20,20,20,20	0
7	CA	A	3717	1/1	1.00	0.16	-	29,29,29,29	0
6	CU	A	500	1/1	1.00	0.02	-	19,19,19,19	1
11	GOL	B	3710	6/6	0.95	0.08	-	24,29,30,31	0
5	MAN	A	3612	11/12	0.79	0.34	-	45,51,53,56	0
6	CU	B	500	1/1	1.00	0.04	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	B	3711	11/12	0.18	0.34	-	98,98,99,99	0
7	CA	A	3713	1/1	1.00	0.03	-	20,20,20,20	0
7	CA	A	3714	1/1	1.00	0.04	-	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.